Agency Dispersion Modeling Capabilities

Jerome D. Fast
Pacific Northwest National Laboratory

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Dispersion Modeling within ASP

Dispersion modeling is performed by scientists in two research programs within the DOE's Atmospheric Sciences Program (ASP):

- ***Environmental Meteorology Program (EMP) - focuses on the transport of energy-related materials through the atmosphere***
- ***Atmospheric Chemistry Program (ACP) - focuses on the chemical transformation of tropospheric energy-related materials on regional, continental, and global scales, the influence of aerosols on air quality and climate, and the characterization and modeling of fine particles***

Models used in EMP and ACP

Three types of models are used within EMP and ACP:

Meteorological Models

- *Mesoscale*
- *Large Eddy Simulation (LES)*
- *Direct Numerical Simulation (DNS)*

Dispersion Models

- *Lagrangian*
- *Eulerian*

Chemical Models

- *Box*
- *Regional*
- *Global*

Meteorological Models

Mesoscale - "widely used codes" within atmospheric community

- *RAMS - CSU Regional Atmospheric Modeling System, MM5 - NCAR/PSU Mesoscale Model, ARPS - OU Advanced Regional Prediction System, ETA - NCEP's operational forecast model*
- *vertical diffusion parameterized for the prognostic momentum, heat, and moisture equations*
- *turbulence parameterization usually based on K-theory and prognostic TKE equation (e.g. Mellor-Yamada closure)*

LES - "research codes"

- *grid ~ 10 - 100 m to resolve small-scale turbulent motions*
- *high frequency end of the turbulence spectrum parameterized*

DNS - "research codes"

- *explicitly resolves turbulence, grid ~ 1 mm*
- *simulations performed using low Re << real atmosphere, but results appear to be independent of Re*

Dispersion Models

Two techniques are used to simulate the transport and diffusion of a passive scalar:

Lagrangian

- *dispersion simulated by tracking a large number of particle positions based on mean and subgrid-scale velocity components*
- *employ the Langevin stochastic differential equation*

Eulerian

- *dispersion simulated by using a continutity equation for a passive scalar on a fixed grid*
- *employ K-theory for vertical diffusion*

Meteorological parameters provided by mesoscale models (also by diagnostic mass-consistent models in the past). Dispersion models are often simply used to identify and illustrate the interaction of various meteorological processes.

Chemical Models

A continuity equation is used for each trace gas specie that includes chemical production/destruction, emission, and deposition terms. K-theory usually employed for vertical diffusion.

high

complexity of chemistry

low

Box

- *"research codes", hundreds of species and reactions*
- *Langrangian, assume air parcel travels with wind*

Regional

- ***STEM*** *(University of Iowa),* ***PEGASUS*** *(PNNL)*
- *meteorological fields imported from mesoscale model at specified intervals (e.g. ~ 1-h intervals)*

Global

- ***IMPACT*** *(LLNL).* ***SUNY-CCM3*** *(SUNY-Albany),* ***MOZART*** *(NCAR),* ***GRANTOUR*** *(UM),* ***GChM*** *(PNNL and BNL)*
- *meteorological fields usually imported from large-scale analyses (e.g. ~ 6-h intervals)*

Model Evaluation

Meteorological Models

- *EMP field campaigns - Brush Creek (1985), Rocky Flats (1991), Mexico City (1997), Salt Lake City (2000)*
- *wind, temperature, humidity averaged over 15 min to 1-h periods from radar wind profilers, sodars, airsondes, and surface stations*

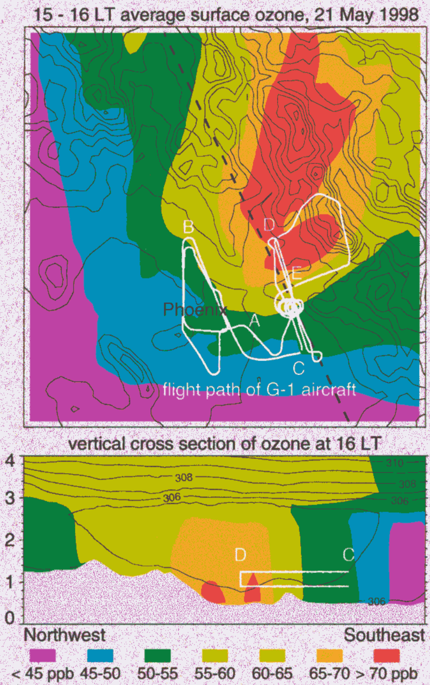
Dispersion Models

- *EMP SF_6 experiments - Brush Creek (1985), Rocky Flats (1991)*
- *hourly average tracer concentrations*

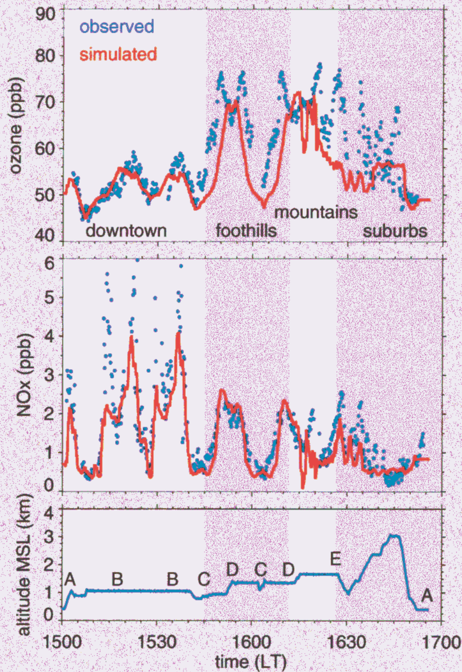
Chemical Models

- *ACP field campaigns - NARE (1992, 93), SOS (1995, 99), NARSTO (1995, 96), Phoenix (1998), NE-OPS (1999), CCOS (2000), TexAQS (2000)*
- *various trace gas species (O_3, NO_x, NO_y, CO, H_2O_2, HCHO, PAN) and aerosols at 10-s intervals or averages over longer periods*
- *surface instrumentation, research aircraft, ozonesondes, and routine air-quality monitoring networks*

Horizontal and Vertical Distribution of Ozone Simulated by PEGASUS



Observed and Simulated Ozone and NOx along G-1 Flight Path



Model Users and Products

EMP and ACP scientists affiliated with:

- *DOE National Laboratories (Argonne, Brookhaven, Laurence Livermore, Los Alamos, and Pacific Northwest)*
- *other government laboratories (NOAA-ATDD, NOAA-ETL, NCAR)*
- *private institutions (Colorado Research Associates, Desert Research Institute)*
- *various universities*

Main objective of EMP and ACP is not to produce models, but to use models to perform basic research reported in

- *peer-reviewed journal articles (special issues)*
- *books*
- *conference proceedings*
- *workshops*

Training Requirements

- *training up to the individual scientists and costs are covered under their own projects*
- *training time depends on the background of individual scientists and the particular model*
- *scientists develop their own code or adapt existing code when necessary to achieve scientific objectives of their projects*

R&D Activities

EMP activities

- *evaluate and improve the representation of topography in mesoscale models and its effect on simulations of vertical exchange processes for urban basins and valleys*
- *evaluate existing subgrid-scale turbulence parameterizations and develop improved treatments for the stable boundary layer*
- *compare simulated turbulence quantities with observations*
- *determine how results from DNS and LES can be "scaled-up" for use in mesoscale models*

ACP activities

- *determine chemical processes within pollutant plumes downwind of point sources (e.g. power plants) and urban areas*
- *fully couple meteorology, gas-phase chemistry, and aerosols to evaluate the effect of feedback processes associated with radiation and clouds*